

Claims

1. A method for routine determination of IC₅₀ or EC₅₀ values for compounds via biological assay at a single concentration, which comprises:

- 5 a) Identifying a biological assay capable of producing a percent effect for a compound tested for activity against a target at a known concentration;
- b) Performing the assay on an initial collection of at least 10 compounds, and at least 1 commercially available compound to be used as positive control, each assayed at a set of 3 to 10 or more concentrations, measuring a
- 10 percent effect at each concentration for each compound;
- c) Determining an IC₅₀ or EC₅₀ for each of these initial compounds by fitting a mathematical dose response curve to the data for each compound, using a computer, and standard linear or nonlinear regression techniques;
- d) Using the resultant data from these initial compounds to fit a
- 15 mathematical relationship between the IC₅₀ or EC₅₀ values and the percent inhibition values at a single fixed concentration X,
- e) Using a computer, and standard linear or nonlinear regression techniques, developing an equation relating IC₅₀ or EC₅₀ to percent inhibition or percent response on all remaining and future test compounds, at the previously fixed
- 20 single concentration X, and determining the IC₅₀ or EC₅₀ via the mathematical equation developed in step d).

2. The method of claim 1 wherein said mathematical dose response curve is the Hill function,

$$\text{percent inhibition} = \frac{100}{1 + \left(\frac{IC_{50}}{\text{concentration}} \right)^h}$$

25 3. The method of claim 1 wherein said mathematical relationship is $IC_{50} = \exp\{a + b \cdot (\text{percent inhibition at concentration } X)\}$.

4. The method of claim 1 wherein said biological assay is an assay for drug-drug interactions related to the target cytochrome P450 (CYP).

5. The method of claim 4 wherein the target is selected from the group consisting of CYP2C9, CYP2D6, CYP3A4, CYP1A2, and CYP2C19.
6. The method of claim 1 where the target is an enzyme.
7. The method of claim 1 wherein the target is a receptor.
- 5 8. The method of claim 1 wherein the target is a transporter.
9. The method of claim 1 wherein said biological assay relates to affinity for any target protein wherein modulation of activity is therapeutically desired.
10. The method of claim 1 wherein said biological assay relates to affinity for any nontherapeutic protein wherein modulation of said activity is undesirable.
- 10